

Advances in Complex Systems
© World Scientific Publishing Company

SPIN-MODELS OF GRANULAR COMPACTION: FROM ONE-DIMENSIONAL MODELS TO RANDOM GRAPHS

JOHANNES BERG

Abdus Salam International Centre for Theoretical Physics, 34100 Trieste, Italy

ANITA MEHTA

*S N Bose National Centre for Basic Sciences, Block JD Sector III, Salt Lake, Calcutta 700 098,
India*

Received (received date)

Revised (revised date)

We discuss two athermal types of dynamics suitable for spin-models designed to model repeated tapping of a granular assembly. These dynamics are applied to a range of models characterised by a 3-spin Hamiltonian aiming to capture the geometric frustration in packings of granular matter.

1. Introduction

Theory and experiment have both contributed extensively to the study of compaction in granular media in recent years. The experiments of the Chicago group [18,19] have in particular inspired a large body of theorists to model the tapping of various systems. In many of these formulations, including the one we present here, an analogy is made between the volume of a granular system and the Hamiltonian of a spin system, along the lines first proposed by Edwards [11]; minimising the energy of the spin system then corresponds to minimising the volume of the granular system.

Grains can interlock only in specific ways, if they are undeformable. It is thus often the case that locally compatible grain orientations could result in globally unfavourable ones, since different (and individually well-packed) clusters of grains could be unfavourably oriented with respect to each other. This frustration is therefore an essential ingredient in the modelling of granular media; it can be modelled in terms of orientational disorder of individual grains [22,15] in lattice-based models, or, as in the present work, the orientational disorder of plaquettes in either lattice or off-lattice models of granular media.

The second ingredient of models of granular compaction is the dynamics designed to model a series of successive taps to the system. A tap applied to a granular assembly for a brief moment feeds kinetic energy into the system and causes

the particles to move with respect to each other. Then the particles fall into a mechanically stable configuration.

In the following sections, we investigate the effect of two model tapping dynamics, called thermal and random tapping, on related models of granular media; the first two of these are on a lattice, while the second is embedded in a structure of random graphs.

2. Random tapping and thermal tapping

A single tap applied briefly to a granular assembly feeds kinetic energy into the system and gives particles the freedom to move with respect to each other, thus momentarily decreasing the density. After this phase, the particles move (subject to gravity) to a new mechanically stable configuration and remain there until perturbed by a further taps. Therefore a recurring theme in modelling taps is the alternation of periods of random perturbation of the system and periods in which the system is allowed to settle into a mechanically stable state.

Models including versions of this principle have included nonsequential Monte Carlo reorganisation schemes [14], lattice-based models of shaken sandboxes [21], the ratio of upward to downward mobility of particles on a lattice [8], or variable rates of absorption and desorption [7].

We now discuss two different ways of transferring this mechanism to spin models, which we will call thermal tapping and random tapping respectively. Both consist of a 'dilation' phase where the system is perturbed at random, and of a quench phase, where the system relaxes after this. The two dynamics differ only in the dilation phase; in both cases the *quench* phase is modelled by a quench of the system at $T = 0$, which lasts until the system has reached a blocked configuration, i.e. each site i has $s_i = \text{sgn}(h_i)$ or $h_i = 0$. Thus at the end of each tap the system will be in a blocked configuration.

In thermal tapping [5] the dilation phase is modelled by a single sequential Monte-Carlo-sweep of the system at a dimensionless temperature T : A site i is chosen at random and flipped with probability 1 if its spin s_i is antiparallel to its local field h_i or $h_i = 0$ and with probability $\exp(-h_i/T)$ if it is not. This procedure is repeated N times.

In random tapping [4,9,10], however, the dilation phase consists in flipping a certain fraction p of randomly chosen spins, regardless of the value of their local field.

The two dynamics differ only in one point: In the case of thermal tapping, the dynamics during the dilation phase is correlated with the energy landscape. Sites with a large absolute value of the local field h_i have a low probability of flipping into the direction against the field. Such spins may be thought of as being highly constrained by their neighbours, while sites with a low absolute local field correspond to 'loosely constrained' particles.

In the case of random tapping, the configuration reached at the end of the

dilation phase is only one of the many configurations having an overlap $1 - 2p$ with the configuration at the beginning of the tap. The sampling of these configurations, however, is uniform, and not correlated with the energy landscape of the model.

In both cases we use as an initial condition a configuration obtained by quenching the system from a configuration where the spins are chosen independently to be ± 1 with equal probabilities.

3. The ferromagnetic 3-spin Hamiltonian

In this section we discuss a simple Hamiltonian, which, we argue, captures some of the salient features of granular compaction. We consider a 3-spin Hamiltonian where N binary spins $S_i = \pm 1$ interact in triplets

$$H = -\rho N = - \sum_{i < j < k} C_{ijk} S_i S_j S_k \quad (3.1)$$

where the variable $C_{ijk} = 1$ with $i < j < k$ denotes the presence of a plaquette connecting sites i, j, k and $C_{ijk} = 0$ denotes its absence. It has a trivial ground state where all spins point up and all plaquettes are in the configuration $+++$, giving a contribution of -1 to the energy. Yet, *locally*, plaquettes of the type $--+$, $-+-$, $+--$ (satisfied plaquettes) also give the same contribution. This results in a competition between local and global satisfaction of the plaquettes. Locally, any of the satisfied plaquettes are equivalent (thus favouring a paramagnetic state), yet globally a ferromagnetic state may be favoured, since there are few configurations satisfying all plaquettes where 4 configurations $+++$, $--+$, $-+-$, $+--$ occur in equal proportions. In this case, most ground states will be ferromagnetic - corresponding to a state with long-range order and a possibly crystalline state of the granular medium [2,3,16].

However *two* spin flips are required to take a given plaquette from one satisfied configuration to another. Thus an energy barrier has to be crossed in any intermediate step between two satisfied configurations. In the context of granular matter, this mechanism aims to model the situation where compaction follows a temporary dilation; for example, a grain could form an unstable ('loose') bridge with other grains before it collapses into an available void beneath the latter. This mechanism, by which an energy barrier has to be crossed in going from one metastable state to another, has recently been argued to be an important ingredient in models of granular compaction [16].

This feature is also shared by models with a two-spin interaction, with transitions e.g. from a state $++$ to $--$. However, in such models domains of a given magnetisation are formed, and the dynamics may be described as the evolution of the walls between these domains. We emphasise that in granular matter, the slow dynamics which is observed experimentally in the regime of high densities, is not necessarily due to the formation of domains; it is in fact due to the extensive number of particle rearrangements which are needed to fill any available voids.

We will see below an instance of this in the 3-spin model we present, where the system remains in a disordered state, with an ongoing slow dynamics; the ordered state is never reached, and domain coarsening to this end is also not observed.

The crucial feature of the model responsible for the slow dynamics is the degeneracy of the four configurations of plaquettes with $s_i s_j s_k = 1$ resulting in a competition between satisfying plaquettes *locally* and *globally*. In the former case, all states with even parity may be used, resulting in a large entropy, while in the latter, only the $+++$ state may be used. A dynamics based on local quantities will thus *fail* to find the magnetised configurations of low energy.

This mechanism has a suggestive analogy with the concept of geometrical frustration in granular matter, if we think of plaquettes as granular clusters. When grains are shaken, they rearrange locally, but locally dense configurations can be mutually incompatible. Voids may appear between densely packed clusters as a consequence of these mutually incompatible cluster orientations, leading to a decrease in the global packing fraction of the assembly. The process of compaction in granular media can in this sense be viewed as an optimisation process involving the competition between the compaction of *local* clusters and the simultaneous minimisation of voids *globally*.

4. One-dimensional models

We first introduce two *one-dimensional* variants of the ferromagnetic 3-spin Hamiltonian as toy models; these illustrate some properties of the 3-spin Hamiltonian as well as the difference between random and thermal tapping.

The first one (model A) simply bunches 3 successive spins to a plaquette, so

$$H = - \sum_i s_i s_{i+1} s_{i+2} \quad (4.1)$$

with cyclic boundary conditions. The statistical mechanics of this model is trivial; it has a transfer matrix

$$T = \begin{pmatrix} e^\beta & 0 & e^{-\beta} & 0 \\ e^{-\beta} & 0 & e^\beta & 0 \\ 0 & e^{-\beta} & 0 & e^\beta \\ 0 & e^\beta & 0 & e^{-\beta} \end{pmatrix} \quad (4.2)$$

with the largest eigenvalue equal to $2 \cosh(\beta)$. A thermal dynamics at finite temperature will thus reveal a paramagnet, with a transition to one of the four ground-states $+++++\dots$, $+-+-+-\dots$, $--+--+--\dots$, $-+-+-+-\dots$ (the latter 3 being related by translation) at $T = 0$. The obvious problem with this Hamiltonian for modelling shaken granular media is that one-flip stable states, which arise where there is a single frustrated plaquette, are also domain walls between neighbouring segments of one of the 4 (ordered) ground states, which we have argued are not the dominant defects impeding the compaction of granular media.

This is remedied to a certain extent in the second model (model B), which consists of 3 threads of ferromagnetically interacting spins, which are in turn linked by a three-spin interaction

$$H = - \sum_{i,a} s_i^a s_{i+1}^a - J \sum_i s_i^1 s_i^2 s_i^3, \quad (4.3)$$

where a , which labels the thread, runs from 1 to 3. Again there are four ground states consisting of three lines with all spins up, or two lines with all spins down and one with all spins up. For $J > 2$ there are now excitations involving a single position only, such as the one shown in figure 1, which are stable against single spin flips.

The entries of the transfer-matrix of this model are $\langle s^1 s^2 s^3 | T | q^1 q^2 q^3 \rangle = \exp\{\beta J s^1 s^2 s^3 + \beta(s^1 q^1 + s^2 q^2 + s^3 q^3)\}$ with the largest eigenvalue equal to $1/2e^{-\beta(6+J)}(3e^{5\beta} + e^{9\beta} + 3e^{\beta(5+2J)} + e^{\beta(9+2J)} + \sqrt{e^{10\beta}(3 + e^{4\beta})(1 + e^{2\beta})^2 + 4e^{2\beta(3+J)}(1 - e^{4\beta})})$.

Under a thermal dynamics, and given a sufficiently slow rate of decreasing the temperature, both models reach equilibrium. After a single quench, models A and B reach a density (termed the single particle relaxation threshold (SPRT) in [4]) found to be ~ 0.63 (this coincides with the result for the corresponding 2-spin model, see [9,10]). Both systems under further thermal tapping show a very slow increase of the density (decrease of the energy) towards the ground state, as shown in figures 2 and 3 respectively. Under random tapping, however, no increase of the density is observed beyond that reached by a single quench in either of models A and B.

For model A, the reason for this behaviour is straightforward. In the case of the 2-spin (Ising) model, a domain wall may be moved with a single spin flip of zero energy. In the case of model A, however, a shift of the domain wall by one lattice site will result in a new frustrated plaquette, and only a further shift will restore the energy to its previous value. This mechanism is illustrated in figure 4. It is clear that a random tapping dynamics thus cannot efficiently move domains, which is a necessary step in domain growth as well as the annihilation of smaller domains. The dilation phase of a thermal tap, on the other hand, is a mechanism by which domain walls may be moved.

The same line of argument holds for model B, where, for example, it takes four

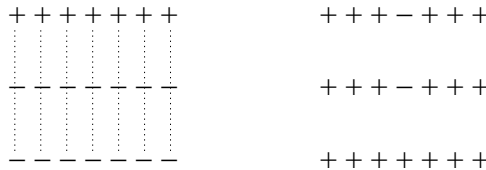


Fig. 1. Left: A ground state of model B. The 3-spin interactions are indicated by the dotted lines. Right: An excited state, which for $J > 2$ is stable against single spin-flips.

flips and a temporary expense of energy, to move the defect shown in figure 1. As discussed in section 3, the mechanism of the system having to expend energy (i.e. lower the density) before being able to move to a new state of lower or equivalent energy, is one of the main motivations for the use of the 3-spin Hamiltonian.

5. The random graph model

We now turn to a different manifestation of the ferromagnetic 3-spin Hamiltonian and consider (3.1) on a random graph.

A random graph [6] consists of a set of nodes and bonds, with the bonds connecting each node at random to a finite number of others, thus from the point of view of connectivity appearing like a finite-dimensional structure. Each bond may link up two sites (a graph) or more (a so-called hypergraph).

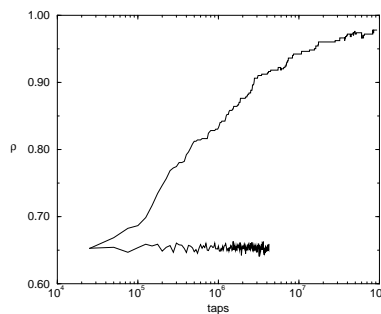


Fig. 2. We compare thermal and random tapping for the 3spin model A. Whereas thermal tapping reaches the highest density (ordered state), random tapping does not take the system beyond the density reached by a single quench. We use $\rho = -H$ and the data stem from a system of size $N = 1002$ with $p = .01$ in the case of random tapping and $T = 1/3$, in the case of thermal tapping. Different values of p give qualitatively the same result.

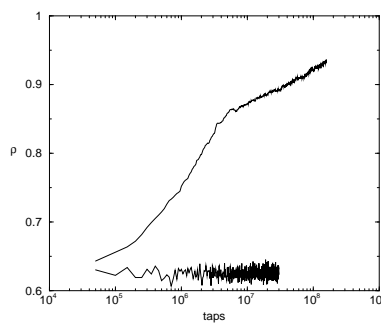


Fig. 3. Model B also shows different behaviour for random and for thermal tapping; only thermal tapping takes the system to densities larger than that reached by a single quench (single particle relaxation threshold). We use $\rho = -H/8$ and $J = 5$ and a system of size $N = 1002$ with $p = .01$ in the case of random tapping, with $T = 1$ in the case of thermal tapping.

In a similar fashion, graphs – strictly speaking hypergraphs – with plaquettes connecting 3 or more nodes each, may be constructed. Choosing the connectivity matrix in the Hamiltonian (3.1) $C_{ijk} = 1(0)$ randomly with probability $2c/N^2$ ($1 - 2c/N^2$), results in a random 3-hypergraph, where the number of plaquettes connected to a site is distributed with a Poisson distribution of average c .

In the context of modelling the compaction of granular matter, random graphs are the simplest structures with a finite number of neighbours. This finite connectivity is a key property, which goes beyond the simple fact that the grains in a deposit are in contact with a finite number of neighbouring grains. E. g. cascades found experimentally during the compaction process may be explained by interactions between a finite number of neighbouring sites, where one local rearrangement sets off another one in its neighbourhood, and so on [4].

Another reason for the use of random graphs lies in the disordered structure of granular matter even at high densities. A random graph is the simplest object where a neighbourhood of each site may be defined, without the consequent appearance of global symmetries such as would appear in the case of a regular lattice. Additionally, the locally fluctuating connectivity may be thought of as modelling the range of coordination numbers of the grains [1].

The absence of domains and domain walls in this case stems of course from the lack of spatial structure. Nevertheless, in the case of the Hamiltonian (3.1), there is an ordered ground state corresponding to all spins being up.

The behaviour of this model under both random and thermal tapping has been described in [4] and [5], respectively. We briefly recapitulate the results and then discuss the difference between the two dynamics in this case.

The dynamical behaviour may be divided into three regimes. The first one only lasts for the duration of a single tap, and consists of the alignment of all spins with their local field. The density reached by this process has been termed the single particle relaxation threshold (SPRT) [4].

In the second regime, which we term the compaction phase, the system seeks

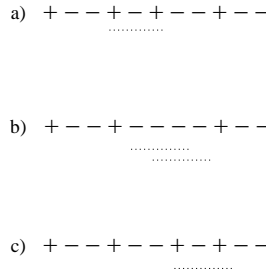


Fig. 4. a) A domain wall in model A. The frustrated plaquette is marked by the dotted line. b) Shifting the domain wall by one step results in the creation of a second frustrated plaquette. c) Only a further shift restores the energy.

to eliminate the remaining frustrated plaquettes. This is a slow process, since at the end of each tap, all spins are aligned with their local fields. The analogy with geometric frustration is that grains are now locally stable and configurations are well packed; in order for any remaining voids to be filled after this, more than one particle around it would have to reorganise. This regime is characterized by a density which increases logarithmically as $\rho(t) \sim \rho(\infty) - a/\log(t)$, with the number of taps. A more detailed expression of this law [18] is

$$\rho(t) = \rho_\infty - (\rho_\infty - \rho_0)/(1 + 1/D \ln(1 + t/\tau)) , \quad (5.1)$$

which may also be written in the simple form $1 + t(\rho)/\tau = \exp \{ D \frac{\rho - \rho_0}{\rho_\infty - \rho} \}$, implying that the dynamics becomes slow (logarithmic) as soon as the density reaches ρ_0 .

The asymptotic density is reached when typical states at this density lie within “valleys” separated by extensive free-energy barriers. Once this density is reached, an extensive number of spins have to be flipped (grains to be moved) to go from one valley to the next, the relaxation time diverges and apart from fluctuations no further compaction occurs. These fluctuations about the asymptotic density mark the third phase of the dynamical behaviour. In spin glasses and spin-models of structural glasses this asymptotic density marks a dynamical phase transition [17, 12]. Configurations with higher densities exist of course, (notably the ferromagnetic ground state corresponding to crystalline order), but a dynamics based on local information will not reach them. In the context of this model, we thus identify the random close packing density with a dynamical transition. Here, the phase space turns from a single, paramagnetic state, into a large number of ‘pockets’ of configurations separated by free-energy barriers, causing a slow dynamics and – at the transition point itself – a breaking of the ergodicity. A simple approximation for the point of the dynamical transition has been given in [20,4,5]. The following figures illustrate the fact that the scenario of a rapid attainment of the SPRT, followed by the logarithmically slow approach to the dynamical transition is borne out both by thermal (figure 5) and by random tapping (figure 6). The two dynamics give similar results in this case, since the irrelevance of geometrical distance on the random graph, does not allow for the presence of domains such as those seen in the previous section. Note that random tapping is, however, much slower in reaching the dynamical threshold. It is important to note also that in both cases, if we increase the tapping intensity, the asymptotic density obtained is below that of the random close packing density corresponding to the dynamic transition [18].

6. Conclusion

Spin models of granular compaction consist of two ingredients: A Hamiltonian, which schematically gives the ‘density’ of the system as a function of the spin configuration, and a dynamics, which aims to model the tapping.

In this paper we discuss the use of 3-spin Hamiltonians, designed to capture the geometrical frustration of grains: locally densely packed configurations may

not be compatible with each other at larger length scales. Also, we discuss two different mechanisms designed to mimic the tapping dynamics of granular matter in the context of spin models. Both consist of alternating periods of increasing and decreasing the energy of the spin system in order to model the dilation and quench phase of individual taps. The two mechanisms differ only in the form of the dilation phase: in thermal tapping this consists of a single Monte-Carlo sweep at a temperature T , whereas in random tapping a fraction p of spins are chosen at random and flipped. These two dynamics were investigated for two different classes of 3-spin Hamiltonians, one-dimensional models and random-graph models. In the latter case, the asymptotic state at low tapping amplitudes (random close packing) corresponds to a dynamical phase transition.

Acknowledgements We thank S. Franz, B. Jones, and M. Sellitto for illuminating discussions.

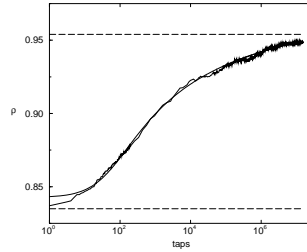


Fig. 5. Compaction curve for thermal tapping at connectivity $c = 3$ for a system of 10^4 spins with $T = .4$. The data stem from a single run and the fit (smooth solid line) follows (5.1) with parameters $\rho_\infty = .989$, $\rho_0 = .843$, $D = 4.716$, and $\tau = 52.46$. The long-dashed line (top) indicates the approximate density 0.954 at which the dynamical transition occurs, the long-dashed line (bottom) indicates the approximate density 0.835 at which the fast dynamics stops, the *single-particle relaxation threshold*.

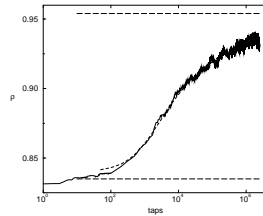


Fig. 6. Compaction curve for random tapping at connectivity $c = 3$ for a system of 10^4 spins (one spin chosen at random is flipped per tap). The data stem from a single run with random initial conditions and the fit (dashed line) follows (5.1) with parameters $\rho_\infty = .971$, $\rho_0 = .840$, $D = 2.76$, and $\tau = 1510$. The long-dashed line (top) indicates the approximate density of the dynamical transition, the long-dashed line (bottom) indicates the approximate density of the single-particle relaxation threshold.

References

- Barker, G. C. and Mehta, A. Vibrated powders: Structure, correlations, and dynamics. *Phys. Rev. A* 45, 3435-3446 (1992).
- [2] Barker G. C. and Mehta, A. Transient phenomena, self-diffusion, and orientational effects in vibrated powders. *Phys. Rev. E* 47, 184-188 (1993).
- [3] Barker G. C. and Mehta, A. Inhomogeneous relaxation in vibrated granular media: consolidation waves. cond-mat/0010268.
- [4] Berg, J. and Mehta, A. On random graphs and the statistical mechanics of granular matter. cond-mat/0012416, to appear in *Europhys. Lett.*
- [5] Berg, J. and Mehta, A. Glassy dynamics in granular compaction: sand on random graphs. cond-mat/0108225, to appear in *Phys. Rev. E*.
- [6] Bollobas B. *Random Graphs*. (Academic Press, London, 1985).
- [7] Brey, J. J., Prados, A. and Sanchez-Rey, B. Simple model with facilitated dynamics for granular compaction. *Phys. Rev. E* 60, 5685-5692 (1999).
- [8] Caglioti, E., Loreto, V., Herrmann, H. J. and Nicodemi, M. A "Tetris-Like" Model for the Compaction of Dry Granular Media. *Phys. Rev. Lett.* 79, 1575-1578 (1997).
- [9] Dean, D. S. and Lefèvre, A. Tapping Spin Glasses and Ferromagnets on Random Graphs. *Phys. Rev. Lett.* 86, 5639-5642 (2001),
- [10] Lefèvre, A. and Dean, D. S. Tapping Thermodynamics of the One Dimensional Ising Model. *J. Phys. A* 34 (14) L213-L220 (2001),
- [11] Edwards, S. F. The role of entropy in the specification of a powder in *Granular Matter: An Interdisciplinary Approach*, (A. Mehta, ed.), New York: Springer-Verlag (1994).
- [12] Franz, S. and Parisi, G. Recipes for Metastable States in Spin-Glasses. *J. Physique I* 5, 1401-1502 (1995).
- [13] Kob, W. and Andersen, H. C. Kinetic lattice-gas model of cage effects in high-density liquids and a test of mode-coupling theory of the ideal-glass transition. *Phys. Rev. E* 48, 4364-4377 (1993).
- [14] Mehta, A. and Barker, G. C. Vibrated powders: A microscopic approach. *Phys. Rev. Lett.* 67, 394-397 (1991).
- [15] Mehta, A. and Barker, G. C. Disorder, memory and avalanches in sand-piles *Europhysics Lett.* 27, 501-506 (1994).
- [16] Mehta, A. and Barker, G. C. Glassy dynamics in granular compaction. *J. Phys. C* 12, 6619-6628, (2000).
- [17] Monasson, R. Structural Glass Transition and the Entropy of the Metastable States. *Phys. Rev. Lett.* 75, 2847-2850 (1995).
- [18] Nowak, E. R., Knight, J., Ben-Naim, E., Jaeger, H. and Nagel, S. R. Density fluctuations in vibrated granular materials *Phys. Rev. E* 57(2), 1971-1982 (1998).
- [19] Nowak, E. R., Knight, J. B., Povinelli, M., Jaeger, H. M. and Nagel, S. R. Reversibility and irreversibility in the packing of vibrated granular material. *Powder Technology* 94, 79-83 (1997).
- [20] Ricci-Tersenghi, F., Weigt, M. and Zecchina, R. Simplest random K-satisfiability problem. *Phys. Rev. E* 63, 026702-026713 (2001).
- [21] Stadler, P. F., Mehta, A., and Luck, J. M. Shaking a Box of Sand. cond-mat/0103076, to appear in *Europhys. Lett.*
- [22] Stadler, P., Mehta, A., and Luck, J. M., 'Glassy states in a shaken sandbox'. in this volume